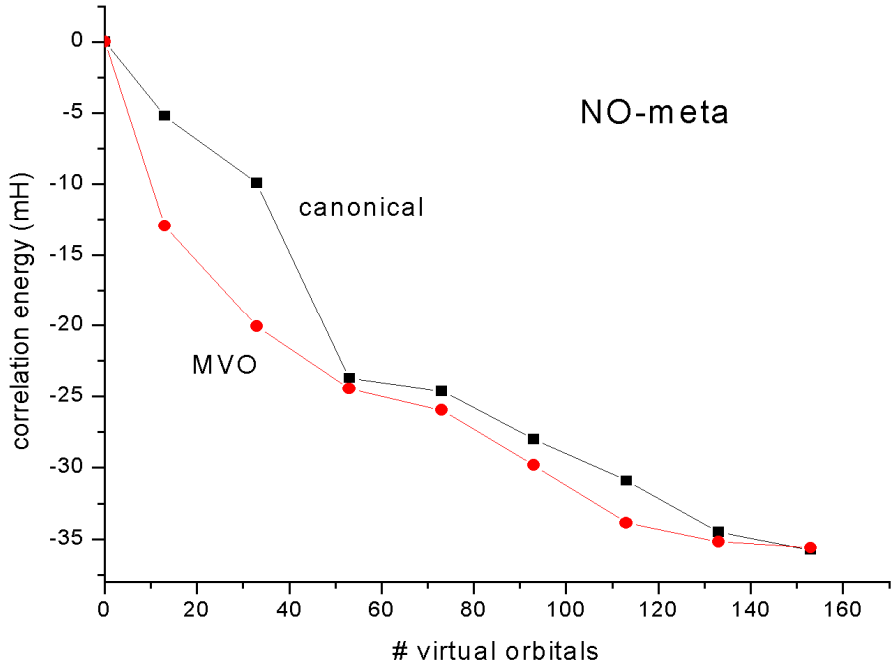
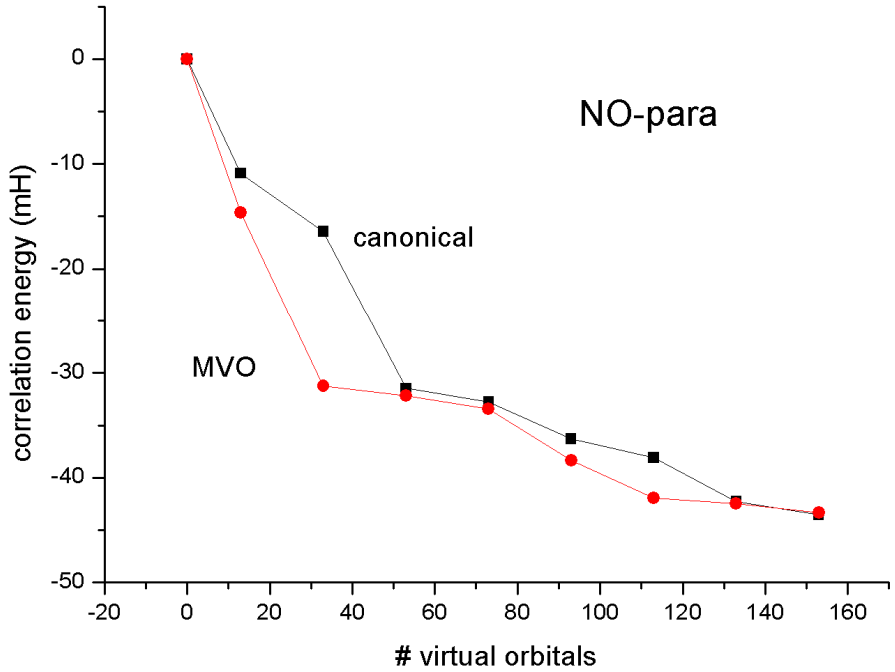
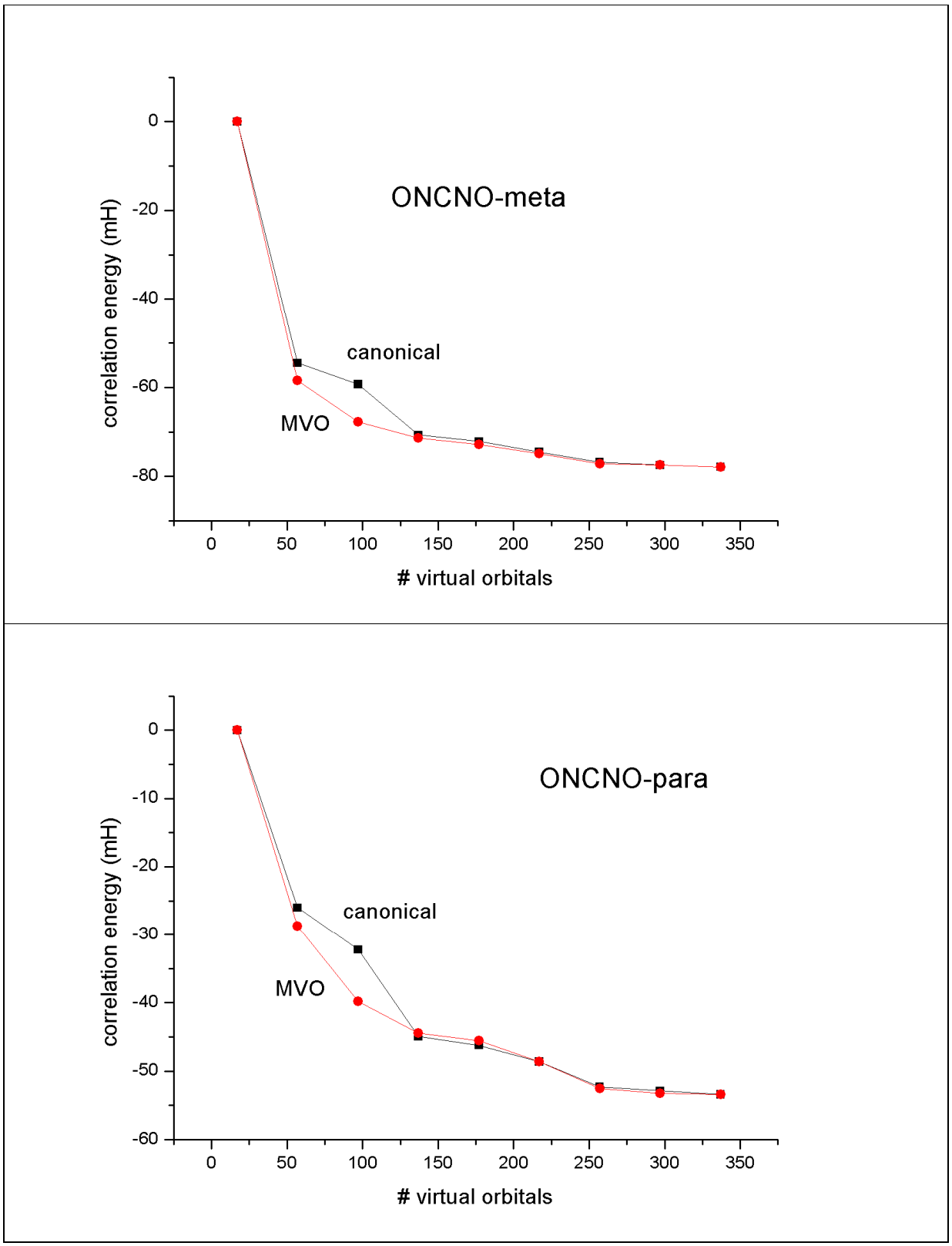
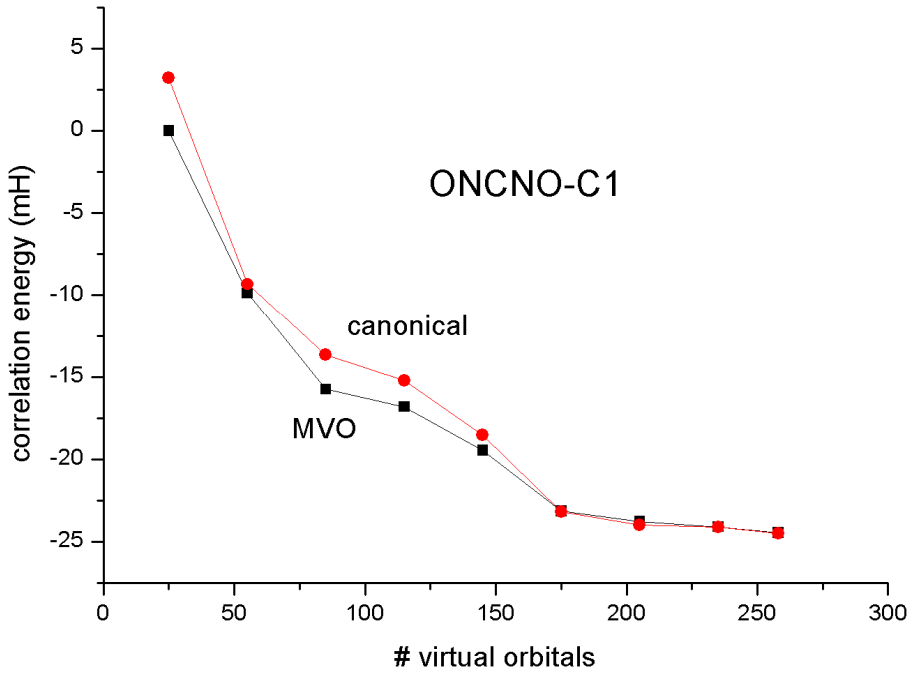
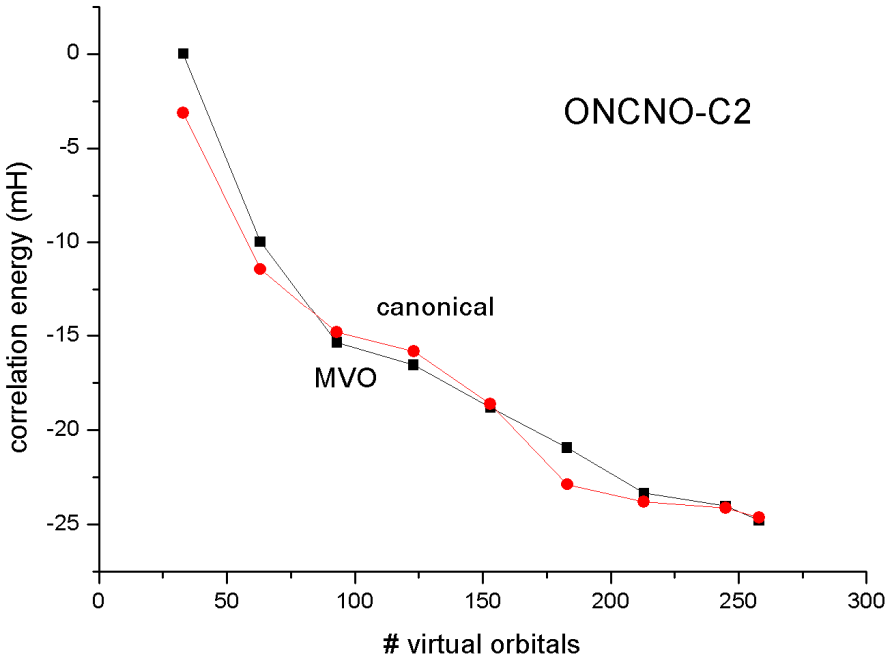
Correlation energy of the considered systems: comparison between canonical orbitals and MVOs.

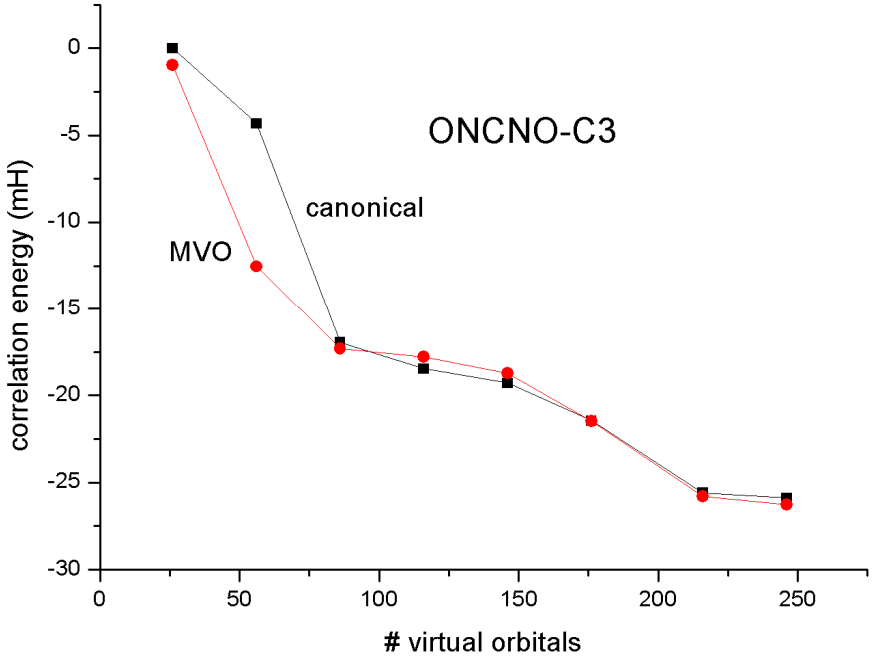





ONCNO-meta
correlation energy (mH)
0
-20
-40
-60
-80
canonical
MVO
0
50
100
150
200
250
300
350
virtual orbitals
ONCNO-para
correlation energy (mH)
0
-10
-20
-30
-40
-50
-60
canonical
MVO
0
50
100
150
200
250
300
350
virtual orbitals


ONCNO-C1
correlation energy (mH)
virtual orbitals
canonical
MVO
5
0
-5
-10
-15
-20
-25
0
50
100
150
200
250
300


ONCNO-C2
correlation energy (mH)
virtual orbitals
canonical
MVO
0
-5
-10
-15
-20
-25
0
50
100
150
200
250
300


ONCNO-C3
canonical
MVO
correlation energy (mH)
virtual orbitals
0
-5
-10
-15
-20
-25
-30
0
50
100
150
200
250

In this graph we present the small changes that can be achieved by using slightly different extra charges on the nuclei bearing unpaired electrons. As an example we report the NO-para system. The sisnglet-triplet energy gap is reported vs. the number of virtual orbitals employed in the DDCI2 calculations, for three set of virtual orbitals.
1- canonical MOs
2 – MVO obtained with extra charge 1.0*e* on all N and O nuclei.
3 – MVO obtained with extra charge 0.9*e* on all N nuclei and 1.1*e* on all O nuclei.

The case 3 with respect to the case 3, shows a small improvements for low number of virtual orbitals, although for 120 MVOs slightly worse results are observed.

Other possible nuclear extra charges lead to worse results.